Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 07:56 AM EDT

PDB ID	:	1GLB
Title	:	STRUCTURE OF THE REGULATORY COMPLEX OF ESCHERICHIA COLI IIIGLC WITH GLYCEROL KINASE
Authors	:	Hurley, J.H.; Worthylake, D.; Faber, H.R.; Meadow, N.D.; Roseman, S.; Pettigrew, D.W.; Remington, S.J.
Deposited on	:	1992-10-28
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

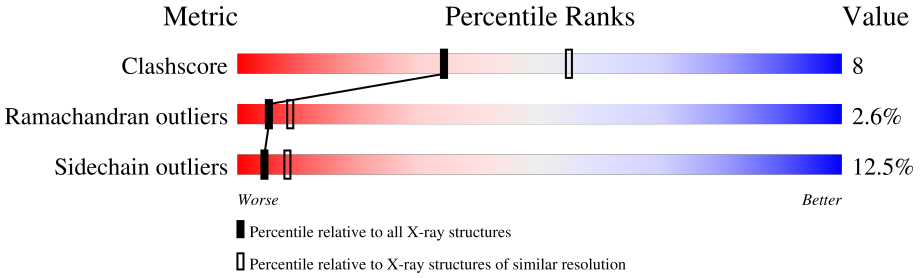
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	F	168	69% 26% • •
2	G	501	64% 27% 6% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5018 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

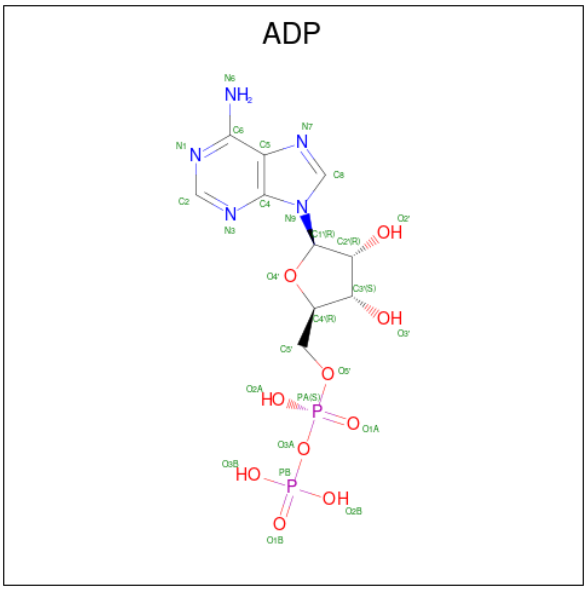
- Molecule 1 is a protein called GLUCOSE-SPECIFIC PROTEIN IIIGlc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	162	1202	769	191	240	2	0	0	1

- Molecule 2 is a protein called GLYCEROL KINASE.

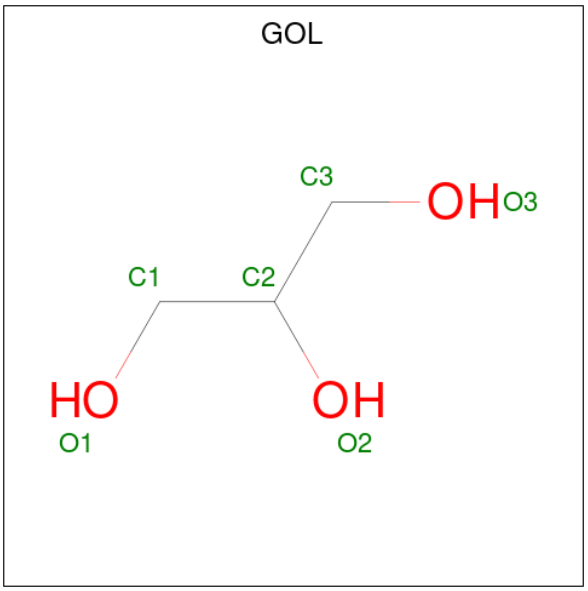
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	490	3783	2387	655	722	19	0	0	1

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	G	1	27	10	5	10	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	G	1	6	3	3	0	0

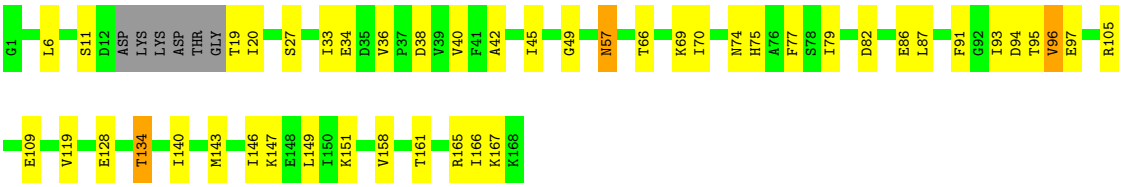
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

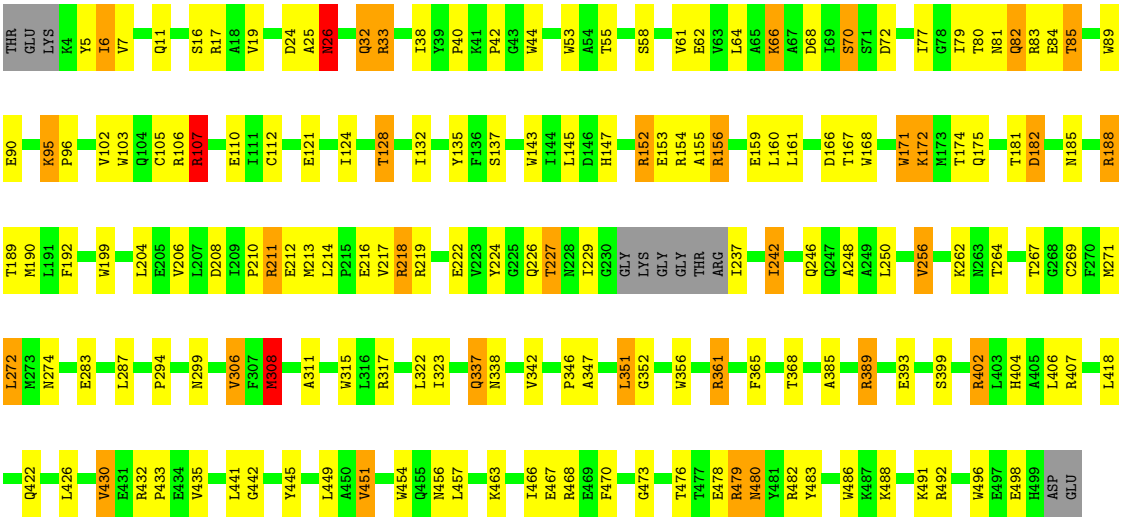
- Molecule 1: GLUCOSE-SPECIFIC PROTEIN IIIGlc

Chain F:



- Molecule 2: GLYCEROL KINASE

Chain G:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.70Å 124.90Å 134.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.205 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5018	wwPDB-VP
Average B, all atoms ($Å^2$)	24.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	F	0.71	0/1217	1.39	7/1647 (0.4%)
2	G	0.80	0/3861	1.60	79/5251 (1.5%)
All	All	0.78	0/5078	1.56	86/6898 (1.2%)

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	188	ARG	NE-CZ-NH1	10.90	125.75	120.30
2	G	83	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	G	199	TRP	CD1-CG-CD2	8.75	113.30	106.30
2	G	361	ARG	NE-CZ-NH1	8.42	124.51	120.30
2	G	496	TRP	CD1-CG-CD2	8.40	113.02	106.30
2	G	445	TYR	CB-CG-CD2	-8.30	116.02	121.00
2	G	454	TRP	CD1-CG-CD2	7.88	112.61	106.30
2	G	199	TRP	CE2-CD2-CG	-7.86	101.01	107.30
2	G	171	TRP	CD1-CG-CD2	7.82	112.56	106.30
2	G	315	TRP	CD1-CG-CD2	7.68	112.44	106.30
2	G	107	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	G	89	TRP	CD1-CG-CD2	7.59	112.38	106.30
2	G	44	TRP	CD1-CG-CD2	7.57	112.36	106.30
2	G	496	TRP	CE2-CD2-CG	-7.54	101.27	107.30
2	G	486	TRP	CE2-CD2-CG	-7.52	101.29	107.30
2	G	83	ARG	NE-CZ-NH2	-7.38	116.61	120.30
2	G	317	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	G	315	TRP	CE2-CD2-CG	-7.25	101.50	107.30
2	G	103	TRP	CE2-CD2-CG	-7.19	101.55	107.30
2	G	156	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	F	57	ASN	N-CA-C	7.15	130.30	111.00
2	G	53	TRP	CE2-CD2-CG	-7.15	101.58	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	486	TRP	CD1-CG-CD2	7.12	112.00	106.30
2	G	454	TRP	CE2-CD2-CG	-7.10	101.62	107.30
2	G	53	TRP	CD1-CG-CD2	7.05	111.94	106.30
2	G	103	TRP	CD1-CG-CD2	6.98	111.89	106.30
2	G	89	TRP	CE2-CD2-CG	-6.96	101.73	107.30
2	G	168	TRP	CE2-CD2-CG	-6.89	101.79	107.30
2	G	143	TRP	CE2-CD2-CG	-6.80	101.86	107.30
2	G	171	TRP	CE2-CD2-CG	-6.75	101.90	107.30
2	G	168	TRP	CD1-CG-CD2	6.59	111.58	106.30
2	G	356	TRP	CD1-CG-CD2	6.57	111.55	106.30
2	G	44	TRP	CE2-CD2-CG	-6.56	102.06	107.30
2	G	143	TRP	CD1-CG-CD2	6.54	111.53	106.30
2	G	407	ARG	NE-CZ-NH2	-6.48	117.06	120.30
2	G	356	TRP	CE2-CD2-CG	-6.45	102.14	107.30
2	G	106	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	F	165	ARG	NE-CZ-NH2	-6.31	117.15	120.30
2	G	389	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	G	135	TYR	CB-CG-CD2	-6.05	117.37	121.00
2	G	308	MET	N-CA-CB	-6.03	99.75	110.60
2	G	103	TRP	CG-CD2-CE3	5.92	139.23	133.90
2	G	147	HIS	CA-CB-CG	-5.91	103.56	113.60
2	G	152	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	G	242	ILE	CB-CA-C	-5.82	99.97	111.60
2	G	152	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	G	199	TRP	CB-CG-CD1	-5.73	119.55	127.00
2	G	219	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	G	491	LYS	CA-CB-CG	5.69	125.92	113.40
2	G	482	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	G	89	TRP	CG-CD2-CE3	5.65	138.98	133.90
2	G	486	TRP	CG-CD2-CE3	5.63	138.97	133.90
2	G	5	TYR	CB-CG-CD2	-5.58	117.65	121.00
2	G	103	TRP	CB-CG-CD1	-5.55	119.79	127.00
2	G	199	TRP	CG-CD2-CE3	5.53	138.87	133.90
2	G	106	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	G	323	ILE	N-CA-C	5.50	125.84	111.00
2	G	492	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	G	211	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	G	457	LEU	N-CA-C	5.42	125.64	111.00
2	G	430	VAL	CG1-CB-CG2	-5.42	102.23	110.90
2	G	199	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	F	70	ILE	N-CA-C	-5.41	96.40	111.00
2	G	68	ASP	CA-C-N	-5.40	105.32	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	496	TRP	CG-CD1-NE1	-5.37	104.73	110.10
2	G	361	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	G	451	VAL	N-CA-CB	-5.30	99.83	111.50
1	F	109	GLU	CA-C-N	5.29	126.78	116.20
2	G	317	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	G	271	MET	CG-SD-CE	-5.28	91.76	100.20
2	G	53	TRP	CB-CG-CD1	-5.27	120.15	127.00
2	G	322	LEU	CA-C-N	5.27	128.80	117.20
2	G	272	LEU	CA-CB-CG	5.26	127.39	115.30
1	F	134	THR	CA-CB-CG2	5.23	119.72	112.40
2	G	337	GLN	CB-CA-C	-5.22	99.97	110.40
2	G	44	TRP	CG-CD1-NE1	-5.19	104.91	110.10
2	G	402	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	G	89	TRP	CB-CG-CD1	-5.19	120.26	127.00
2	G	483	TYR	CB-CG-CD2	-5.14	117.91	121.00
2	G	468	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	G	53	TRP	CG-CD2-CE3	5.13	138.52	133.90
1	F	87	LEU	CA-CB-CG	5.08	126.99	115.30
2	G	496	TRP	CB-CG-CD1	-5.08	120.40	127.00
2	G	156	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	F	38	ASP	CA-C-N	-5.01	106.17	117.20
2	G	337	GLN	N-CA-CB	5.00	119.61	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1202	0	1217	20	0
2	G	3783	0	3637	64	0
3	G	27	0	12	0	0
4	G	6	0	8	0	0
All	All	5018	0	4874	83	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:ILE:HD12	1:F:166:ILE:HD11	1.59	0.82
2:G:33:ARG:HG3	2:G:55:THR:HG22	1.72	0.71
1:F:40:VAL:HA	1:F:45:ILE:HD12	1.74	0.70
1:F:143:MET:SD	1:F:146:ILE:HD11	2.33	0.68
2:G:137:SER:HB2	2:G:189:THR:HA	1.79	0.64
2:G:26:ASN:HD22	2:G:26:ASN:H	1.43	0.64
2:G:7:VAL:HB	2:G:77:ILE:HD13	1.80	0.63
2:G:256:VAL:HG13	2:G:294:PRO:HG3	1.82	0.62
2:G:476:THR:O	2:G:479:ARG:HB2	2.00	0.61
2:G:85:THR:HB	2:G:102:VAL:HA	1.81	0.61
2:G:269:CYS:HB2	2:G:306:VAL:HG22	1.81	0.61
2:G:274:ASN:HD21	2:G:299:ASN:HD22	1.49	0.60
2:G:227:THR:HG22	2:G:237:ILE:HA	1.83	0.60
1:F:74:ASN:HD21	1:F:105:ARG:HD2	1.68	0.59
1:F:75:HIS:HD2	1:F:95:THR:HB	1.66	0.58
1:F:74:ASN:ND2	1:F:105:ARG:HD2	2.18	0.58
2:G:58:SER:O	2:G:62:GLU:HB2	2.04	0.57
2:G:248:ALA:O	2:G:442:GLY:HA3	2.05	0.56
2:G:81:ASN:ND2	2:G:166:ASP:HB3	2.22	0.55
2:G:267:THR:HG23	2:G:311:ALA:HB2	1.87	0.55
2:G:38:ILE:HG22	2:G:40:PRO:HD3	1.88	0.55
2:G:62:GLU:O	2:G:66:LYS:HB2	2.07	0.55
2:G:192:PHE:HE1	2:G:217:VAL:HG11	1.72	0.54
2:G:154:ARG:HG2	2:G:159:GLU:HB2	1.90	0.53
2:G:430:VAL:HB	2:G:470:PHE:HB2	1.89	0.53
1:F:34:GLU:HA	1:F:42:ALA:HA	1.90	0.53
2:G:174:THR:HG22	2:G:226:GLN:O	2.08	0.53
2:G:105:CYS:SG	2:G:107:ARG:HB3	2.49	0.53
1:F:94:ASP:O	1:F:97:GLU:HG2	2.08	0.52
2:G:105:CYS:SG	2:G:107:ARG:NH1	2.82	0.52
2:G:128:THR:HG21	2:G:190:MET:HA	1.90	0.52
2:G:422:GLN:NE2	2:G:426:LEU:HD13	2.25	0.52
1:F:69:LYS:O	1:F:77:PHE:HA	2.09	0.52
1:F:74:ASN:ND2	1:F:105:ARG:HB2	2.25	0.51
1:F:75:HIS:CD2	1:F:95:THR:HB	2.43	0.51
2:G:64:LEU:HD22	2:G:70:SER:HA	1.93	0.51
2:G:156:ARG:HA	2:G:212:GLU:OE1	2.11	0.50
1:F:74:ASN:HD21	1:F:105:ARG:HH11	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:182:ASP:HB3	2:G:242:ILE:HB	1.94	0.49
2:G:128:THR:HG23	2:G:192:PHE:O	2.12	0.49
2:G:189:THR:O	2:G:190:MET:HB3	2.13	0.49
2:G:211:ARG:HG3	2:G:214:LEU:HD12	1.95	0.48
2:G:435:VAL:HG11	2:G:441:LEU:HD11	1.96	0.47
2:G:422:GLN:O	2:G:426:LEU:HB2	2.13	0.47
1:F:96:VAL:HG21	2:G:478:GLU:HG2	1.96	0.47
2:G:171:TRP:CE3	2:G:172:LYS:HE2	2.50	0.47
2:G:246:GLN:HB3	2:G:272:LEU:HD11	1.96	0.47
2:G:153:GLU:HA	2:G:156:ARG:HH11	1.79	0.46
2:G:171:TRP:HE3	2:G:172:LYS:HE2	1.81	0.46
1:F:20:ILE:HB	1:F:166:ILE:HG13	1.98	0.45
1:F:77:PHE:CZ	1:F:119:VAL:HG21	2.52	0.45
2:G:155:ALA:CB	2:G:210:PRO:HG3	2.47	0.45
2:G:435:VAL:HG11	2:G:441:LEU:CD1	2.46	0.45
2:G:385:ALA:HA	2:G:422:GLN:OE1	2.17	0.45
2:G:389:ARG:HH12	2:G:479:ARG:HG2	1.82	0.45
2:G:347:ALA:HB2	2:G:351:LEU:HD13	1.99	0.44
2:G:308:MET:HB2	2:G:346:PRO:HB2	1.98	0.44
1:F:140:ILE:HD12	1:F:149:LEU:HD11	1.99	0.44
2:G:82:GLN:OE1	2:G:85:THR:HG21	2.17	0.44
2:G:188:ARG:HH22	2:G:287:LEU:HD13	1.83	0.44
2:G:210:PRO:HG2	2:G:213:MET:HG3	2.00	0.44
2:G:347:ALA:O	2:G:361:ARG:HA	2.18	0.44
2:G:152:ARG:HD3	2:G:208:ASP:OD2	2.18	0.43
2:G:264:THR:O	2:G:269:CYS:HA	2.19	0.43
2:G:152:ARG:HG2	2:G:156:ARG:NH1	2.33	0.43
2:G:308:MET:H	2:G:308:MET:HG2	1.64	0.43
2:G:16:SER:O	2:G:32:GLN:HA	2.19	0.43
2:G:26:ASN:H	2:G:26:ASN:ND2	2.15	0.42
2:G:402:ARG:HE	2:G:404:HIS:HE1	1.67	0.42
2:G:480:ASN:HD22	2:G:480:ASN:N	2.17	0.42
1:F:49:GLY:O	1:F:151:LYS:HE3	2.20	0.42
2:G:112:CYS:HB3	2:G:132:ILE:HG22	2.00	0.42
2:G:155:ALA:HB2	2:G:160:LEU:HD11	2.02	0.42
2:G:342:VAL:HA	2:G:365:PHE:O	2.20	0.42
2:G:432:ARG:HA	2:G:433:PRO:HD2	1.87	0.41
2:G:473:GLY:O	2:G:476:THR:HG22	2.20	0.41
2:G:250:LEU:HD22	2:G:272:LEU:HD22	2.02	0.41
1:F:66:THR:O	1:F:79:ILE:HG13	2.21	0.41
2:G:6:ILE:HD12	2:G:6:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:SER:OG	1:F:158:VAL:HG12	2.20	0.40
2:G:389:ARG:NH1	2:G:479:ARG:HG2	2.36	0.40
2:G:95:LYS:HA	2:G:96:PRO:HD3	1.91	0.40
1:F:33:ILE:O	1:F:36:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	158/168 (94%)	141 (89%)	15 (10%)	2 (1%)	12 24
2	G	486/501 (97%)	438 (90%)	33 (7%)	15 (3%)	4 6
All	All	644/669 (96%)	579 (90%)	48 (8%)	17 (3%)	5 9

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	57	ASN
2	G	84	GLU
2	G	175	GLN
2	G	229	ILE
2	G	479	ARG
2	G	25	ALA
2	G	222	GLU
2	G	337	GLN
1	F	11	SER
2	G	24	ASP
2	G	463	LYS
2	G	467	GLU
2	G	26	ASN
2	G	218	ARG

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Mol	Chain	Res	Type
2	G	399	SER
2	G	61	VAL
2	G	352	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	133/145 (92%)	121 (91%)	12 (9%)	9 18
2	G	386/412 (94%)	333 (86%)	53 (14%)	3 6
All	All	519/557 (93%)	454 (88%)	65 (12%)	4 8

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	6	LEU
1	F	19	THR
1	F	82	ASP
1	F	86	GLU
1	F	91	PHE
1	F	93	ILE
1	F	96	VAL
1	F	128	GLU
1	F	134	THR
1	F	147	LYS
1	F	161	THR
1	F	167	LYS
2	G	6	ILE
2	G	11	GLN
2	G	17	ARG
2	G	19	VAL
2	G	26	ASN
2	G	32	GLN
2	G	33	ARG
2	G	42	PRO

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Mol	Chain	Res	Type
2	G	66	LYS
2	G	70	SER
2	G	72	ASP
2	G	79	ILE
2	G	80	THR
2	G	82	GLN
2	G	85	THR
2	G	90	GLU
2	G	95	LYS
2	G	107	ARG
2	G	110	GLU
2	G	121	GLU
2	G	124	ILE
2	G	128	THR
2	G	145	LEU
2	G	161	LEU
2	G	167	THR
2	G	172	LYS
2	G	181	THR
2	G	182	ASP
2	G	185	ASN
2	G	204	LEU
2	G	206	VAL
2	G	216	GLU
2	G	218	ARG
2	G	224	TYR
2	G	227	THR
2	G	256	VAL
2	G	262	LYS
2	G	283	GLU
2	G	306	VAL
2	G	308	MET
2	G	338	ASN
2	G	351	LEU
2	G	368	THR
2	G	393	GLU
2	G	406	LEU
2	G	418	LEU
2	G	449	LEU
2	G	451	VAL
2	G	456	ASN
2	G	466	ILE

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Mol	Chain	Res	Type
2	G	480	ASN
2	G	488	LYS
2	G	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	74	ASN
2	G	26	ASN
2	G	32	GLN
2	G	47	HIS
2	G	127	ASN
2	G	253	GLN
2	G	263	ASN
2	G	299	ASN
2	G	404	HIS
2	G	480	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	G	503	-	5,5,5	0.44	0	5,5,5	0.36	0
3	ADP	G	502	-	24,29,29	1.15	3 (12%)	29,45,45	1.10	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	G	503	-	-	0/4/4/4	-
3	ADP	G	502	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	502	ADP	O4'-C1'	2.94	1.44	1.40
3	G	502	ADP	C8-N7	-2.19	1.30	1.34
3	G	502	ADP	PB-O2B	-2.04	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	502	ADP	O3'-C3'-C4'	-2.55	103.75	111.08
3	G	502	ADP	O3B-PB-O3A	-2.04	97.79	104.64

There are no chirality outliers.

There are no torsion outliers.

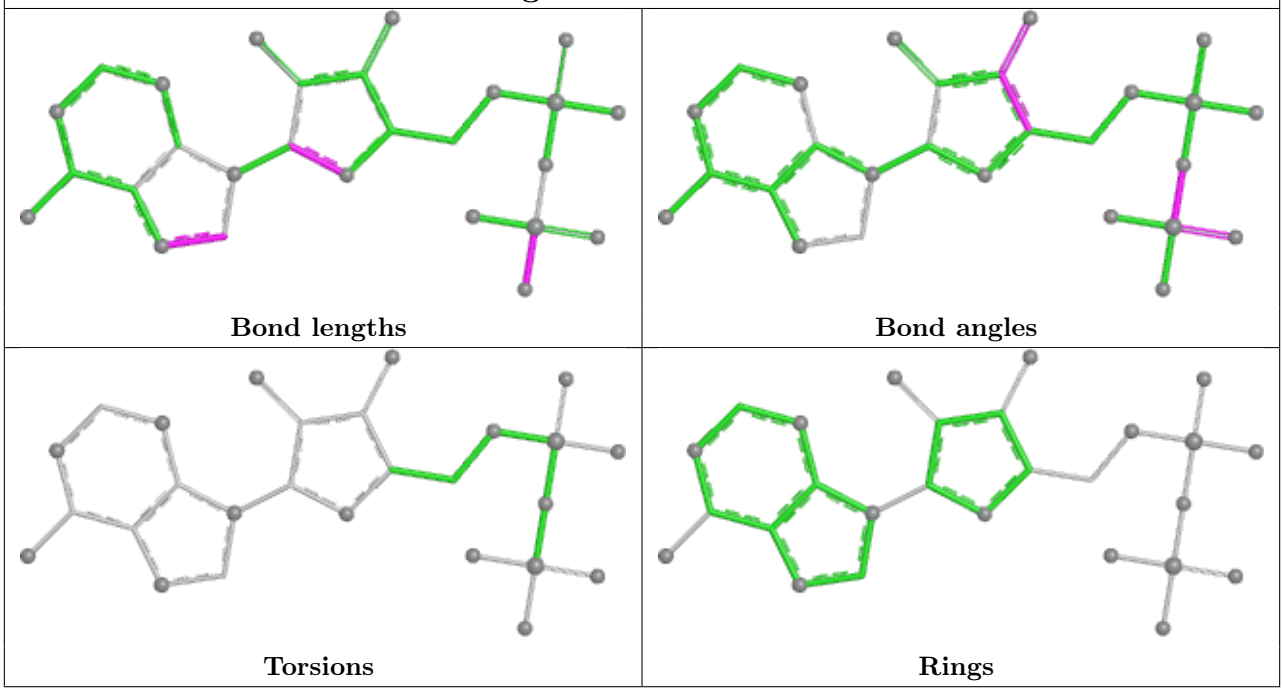
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP G 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.